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ON THE NUMERICAL INFLUENCES OF INERTIA REPRESENTATION FOR RIGID BODY DYNAMICS

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Abstract. *Inertia plays a crucial role in rigid body dynamics, and the associated mass matrix is of various forms in representation. The influences of accuracy of different representation, however, have not drawn enough attention in previous researches about numerical simulation of rigid body dynamics. In the paper, the inertia representation is intensively investigated for rigid body dynamics and a modified formulation is derived through splitting the kinetic energy into two parts: a square term of velocity and a quadratic form in the derivatives with quadratic coefficients in generalized displacement, of which the proportion is controlled by a scaling parameter. Although the kinetic energy with different scaling parameters is theoretically equivalent in dynamics, error estimation demonstrates that accuracy of numerical scheme crucially depends on the particular value of scaling parameter if only rotational coordinates are expressed in pseudo vectors. This attractive feature distinguishes the modified formulation from others in numerical significance. According to the modified representation of inertia, a variational integrator is derived for rigid body dynamics in pseudo vectors. Numerical results demonstrate that the variational integrator, of which the scaling parameter is selected as the arithmetic mean of three principal moments of inertia tensor, is of impressively higher accuracy in simulation, especially compared with the integrations derived with the original formulation of mass matrix.*

1 INTRODUCTION

Rigid body dynamics is applied frequently in engineering, physics, chemistry, molecular dynamics, etc. As well known, the motion of a single body can be split into two separate parts [1], of which, one is the pure translation of a reference point, and the other is pure rotation about the reference point. Although the description and integration of the translation part has found a fairly conclusive form, the rigid body rotation is still actively investigated because a variety of representation coexists and presents their respective advantages in different aspects of the application. The most common and widely used type of rotational coordinates for describing the rotation motion of a rigid body is Euler angles, that one of the minimal representation for rigid body rotation. It has advantage that the motion of rigid body is governed by ordinary differential equations in the description of Euler angle. In the last few decades, the theory of numerical methods for general (non-stiff and stiff) ordinary differential equations has reached a certain maturity [2], excellent general-purpose codes, mainly based on Runge-Kutta methods or linear multistep methods, have become available for the numerical simulation of rigid body dynamics.

Nevertheless, with steady increases in both size and complexity of the systems investigated, pseudo-vectors, such as unit quaternion and convected base vectors, are found new attraction due to the simplicity in mathematical formulation and the possibility of avoiding singularities which may occur in the framework of Euler angles. Because of the non-independence of the parameters in pseudo-vectors, algebraic constraints are usually included in the equations of motion, which essentially extends the equations by holonomic constraints and yields a set of differential-algebraic equations (DAEs) of Index 3, instead of ordinary differential equations (ODEs). According to a formal definition of the index of DAEs [3], the early researches [4-6] underline that higher indices result in more arduous solving process, especially numerical difficulties associated with the solution of these index-3 DAEs. Due to these reasons, a large amount of effort [7-18] has been devoted to the study of computational methods in pseudo-vectors for handling the motion of rigid body.

One of the more remarkable aspects of pseudo-vector is that the inertia representation can greatly influence the numerical accuracy of integrations in simulation. The inertia representation, associated with mass matrix, expresses the connection between velocity of a system and the kinetic energy of that system. Xu and Zhong [19] first found this numerical phenomenon in their research about quaternion-based rigid body dynamics. They present that the quaternion-based mass matrix can be split into two parts: an identity matrix with a scaling parameter, denoted as σ, and a displacement-dependent matrix with a partial inertia tensor, denoted as $\boldsymbol{J}_{\sigma}$, and the proportion of two components is controlled by the scaling parameter. They further demonstrate that geometric integrations with a proper value of scaling parameter is of much higher accuracy than the others. Here we aim to present that the new type of inertia representation are available no matter what kind of rotational coordinates are used to describe the motion of rigid body. In the continuous case these inertia representation with different scaling parameter σ are theoretically equivalent, however, while the pseudo-vector is considered as the rotational coordinates, accuracy of numerical scheme crucially depends on the particular value of scaling parameter that is being chosen as starting point for the discretization process. This attractive feature distinguishes the modified formulation from others in numerical significance. We derive the variational integrator with the aid of the new type of inertia representation. The arithmetic average of three principal moments of inertia, denoted as σ_{m} is recommended as a reasonable preconditioning value of the scaling parameter. Numerical results demonstrate that the variational integrator with $\sigma = \sigma_{\mathrm{m}}$ is of impressively high accuracy, especially compared with the integrator with the original formulation of mass matrix.

2 KINEMATICS

The motion of a single rigid body is illustrated in Figure 1. A body fixed coordinate frame, denoted by *O-XYZ* is centered at point *O* with translation vector $\boldsymbol{x}_0$. A point located inside the rigid body with coordinates $\boldsymbol{X} = [X, Y, Z]^T$ has the global components [18]

$$\boldsymbol{x} = \boldsymbol{x}_0 + \boldsymbol{R}\boldsymbol{X} \tag{1}$$

where $\boldsymbol{R}$ is the rotational matrix satisfying the orthonormal condition

$$\boldsymbol{R}\boldsymbol{R}^T = \boldsymbol{R}^T\boldsymbol{R} = \boldsymbol{I}_3 \tag{2}$$

and $\boldsymbol{I}_3$ is the 3×3 identity matrix.

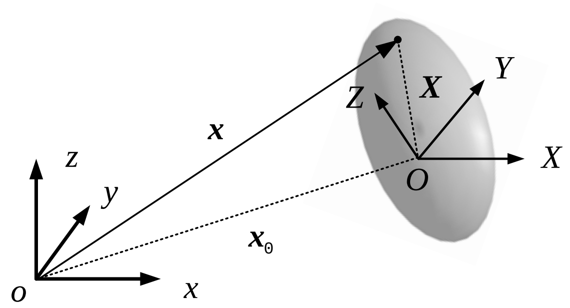

Figure 1: A single body described by translation vector $\boldsymbol{x}_0$ and rotational matrix $\boldsymbol{R}$.

The kinetic energy of a body with volume V_0 can be expressed by the integral

$$T = \frac{1}{2}\int_{V_0} \rho \dot{\boldsymbol{x}}^T \dot{\boldsymbol{x}} \mathrm{d}V_0 \tag{3}$$

where ρ denotes the mass density. Substituting (1) into (3) and selecting the reference point O as the center of mass, the kinetic energy takes a particularly simple form where the translational kinetic energy of the center of mass T_{t} decouples from the rotational kinetic energy of the body T_{r} as

$$T = T_{\mathrm{t}} + T_{\mathrm{r}} \tag{4}$$

First, the translational part of kinetic energy of the mass center is expressed as

$$T_{\mathrm{t}} = \frac{1}{2} m \dot{\boldsymbol{x}}_0^T \dot{\boldsymbol{x}}_0 \tag{5}$$

where m denotes the mass of the body, and $\dot{\boldsymbol{x}}_0$ is the velocity of the mass center. Similarly, the rotational part of the kinetic energy can be expressed in terms of the velocity $\boldsymbol{v}_{\mathrm{r}}$ due to rotation in the form

$$T_{\mathrm{r}} = \frac{1}{2}\int_{V_0} \rho \boldsymbol{v}_{\mathrm{r}}^T \boldsymbol{v}_{\mathrm{r}} \mathrm{d}V_0 \tag{6}$$

2.1 Rigid body motion

In the present formulation of rotational part of kinetic energy, the vector $\boldsymbol{v}_{\mathrm{r}}$ represents the rotation velocity of a mass point of rigid body in the body fixed coordinate frame $O\text{-}XYZ$. Considered the rigid body is rotating with angular velocity $\boldsymbol{\Omega}$, the rotation velocity can therefore be expressed in terms of the angular velocity $\boldsymbol{\Omega}$ as,

$$\boldsymbol{v}_{\mathrm{r}} = \boldsymbol{\Omega} \times \boldsymbol{X} = \hat{\boldsymbol{\Omega}}\boldsymbol{X} = -\hat{\boldsymbol{X}}\boldsymbol{\Omega} \tag{7}$$

where the symbol ($\wedge$) denotes the vector product via the skew-symmetric local component matrix

$$\hat{\boldsymbol{\Omega}} = \boldsymbol{\Omega}\times = \begin{bmatrix} 0 & -\Omega_3 & \Omega_2 \\ \Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & \Omega_1 & 0 \end{bmatrix} \tag{8}$$

Substituting (7) into (6) yields

$$T_{\mathrm{r}} = \frac{1}{2}\boldsymbol{\Omega}^T \left(\int_{V_0} \rho \hat{\boldsymbol{X}}^T \hat{\boldsymbol{X}} dV_0 \right) \boldsymbol{\Omega} = \frac{1}{2}\boldsymbol{\Omega}^T \boldsymbol{J}\boldsymbol{\Omega} \tag{9}$$

where $\boldsymbol{J}$ is the inertia tensor, defined by the volume integral

$$\boldsymbol{J} = \int_{V_0} \rho \hat{\boldsymbol{X}}^T \hat{\boldsymbol{X}} dV \tag{10}$$

and conveniently expressed in body fixed coordinate frame, whereby $\boldsymbol{J}$ is constant.

Suppose that the angular velocity can be formally expressed as

$$\boldsymbol{\Omega} = \boldsymbol{L}(\boldsymbol{q})^T \dot{\boldsymbol{q}} \tag{11}$$

where $\boldsymbol{q}$ denotes the *n* generalized coordinates described the three dimensional rotation motion and $\dot{\boldsymbol{q}}$ is its velocity; $\boldsymbol{L}(\boldsymbol{q})^T$ represents a geometric mapping between $\boldsymbol{\Omega}$ and $\dot{\boldsymbol{q}}$. While $n = 3$, $\boldsymbol{q}$ represents the minimal coordinate representation for rigid body rotation. while $n > 3$, $\boldsymbol{q}$ represents pseudo-vector, of which the *n* components are not independent, and generally *n*-3 constraint equations, defined by

$$\boldsymbol{\psi}(\boldsymbol{q}) = \boldsymbol{0} \tag{12}$$

are imposed on the system to preserve the one to one correspondence relation between $\boldsymbol{\Omega}$ and $\dot{\boldsymbol{q}}$.

The kinetic energy of the rigid body motion can now be expressed in terms of the translation velocity, the generalized coordinates $\boldsymbol{q}$ and the time derivative $\dot{\boldsymbol{q}}$, by substitution of the angular velocity from (11) into the expressions (9), whereby

$$T = \frac{1}{2} m \dot{\boldsymbol{x}}_0^T \dot{\boldsymbol{x}}_0 + \frac{1}{2} \dot{\boldsymbol{q}}^T \boldsymbol{M} \dot{\boldsymbol{q}} \tag{13}$$

where

$$\boldsymbol{M} = \boldsymbol{L}(\boldsymbol{q}) \boldsymbol{J} \boldsymbol{L}(\boldsymbol{q})^T \tag{14}$$

is defined as the mass matrix with respect to the rotation motion.

2.2 Rotational coordinates for rigid body rotation

As presented in the above, the rotational part of kinetic energy can be expressed formally by the generalized coordinates $\boldsymbol{q}$ and the time derivative $\dot{\boldsymbol{q}}$, and however, not every generalized coordinates preserving the one to one mapping relationship between $\boldsymbol{\Omega}$ and $\dot{\boldsymbol{q}}$ can be used to describe the rotation motion of a rigid body. Actually, it can be derived from the infinitesimal rotation that the rotation motion is governed by the differential equations [1]

$$\dot{\boldsymbol{R}} = \boldsymbol{R}\hat{\boldsymbol{\Omega}} \tag{15}$$

Considered that $\boldsymbol{R}^T\boldsymbol{R} = \boldsymbol{I}_3$, we have

$$\hat{\boldsymbol{\Omega}} = \boldsymbol{R}^T\dot{\boldsymbol{R}} \tag{16}$$

which implies a one to one mapping relationship between $\boldsymbol{\Omega}$ and $\dot{\boldsymbol{R}}$, and consequently, it requires one-to-one mapping between $\boldsymbol{q}$ can $\boldsymbol{R}$ to describe the rotation motion of a rigid body with $\boldsymbol{q}$.

1) Euler angles

The most common and widely used type of rotational coordinates is Euler angles. In the description of Euler angles[1], the rotational motion is expressed in terms of the angle of nutation θ, the angle of precession ϕ, and the spin angle ψ, whereby

$$\boldsymbol{R} = \begin{bmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\cos\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\psi\sin\theta \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{bmatrix} \tag{17}$$

Substituting (17) into (16) leads to

$$\begin{aligned} \Omega_1 &= \dot{\phi}\sin\theta\sin\psi + \dot{\theta}\cos\psi \\ \Omega_2 &= \dot{\phi}\sin\theta\cos\psi - \dot{\theta}\sin\psi \\ \Omega_3 &= \dot{\phi}\cos\theta + \dot{\psi} \end{aligned} \tag{18}$$

In combination of (18) with (11), we have the generalized coordinate $\boldsymbol{q} = [\psi, \theta, \phi]^T$ and

$$\boldsymbol{L}(\boldsymbol{q}) = \begin{bmatrix} \sin\theta\sin\psi & \cos\psi & 0 \\ \sin\theta\cos\psi & -\sin\psi & 0 \\ \cos\theta & 0 & 1 \end{bmatrix}^T \tag{19}$$

2) Unit quaternion

Unit quaternion is another popular way to describe the rotation of a rigid body. In the (real) matrix representation [16], unit quaternion can be thought of as a 4-dimensional vector

$$\boldsymbol{q} = [q_0, q_1, q_2, q_3]^T \tag{20}$$

with the unit length constraint

$$\psi(\boldsymbol{q}) = \boldsymbol{q}^T\boldsymbol{q} - 1 = 0 \tag{21}$$

and then the rotation matrix can be expressed in terms of unit quaternion

$$\boldsymbol{R}(\boldsymbol{q})=\begin{bmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(q_1q_2-q_0q_3) & 2(q_1q_3+q_0q_2) \\ 2(q_1q_2+q_0q_3) & q_0^2-q_1^2+q_2^2-q_3^2 & 2(q_2q_3-q_0q_1) \\ 2(q_1q_3-q_0q_2) & 2(q_2q_3+q_0q_1) & q_0^2-q_1^2-q_2^2+q_3^2 \end{bmatrix} \tag{22}$$

Substituting (22) into (16) leads to

$$\begin{aligned} \Omega_1 &= 2(-q_1\dot{q}_0+q_0\dot{q}_1+q_3\dot{q}_2-q_2\dot{q}_3) \\ \Omega_2 &= 2(-q_2\dot{q}_0-q_3\dot{q}_1+q_0\dot{q}_2+q_1\dot{q}_3) \\ \Omega_3 &= 2(-q_3\dot{q}_0+q_2\dot{q}_1-q_1\dot{q}_2+q_1\dot{q}_4) \end{aligned} \tag{23}$$

and correspondingly

$$\boldsymbol{L}(\boldsymbol{q})=2\begin{bmatrix} -q_1 & q_0 & q_3 & -q_2 \\ -q_2 & -q_3 & q_0 & q_1 \\ -q_3 & q_2 & -q_1 & q_0 \end{bmatrix}^T \tag{24}$$

3) Convected base vectors

As an alternative way to describe the rotation of a rigid body, the rotation matrix can be expressed directly by

$$\boldsymbol{R}=[\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3] \tag{25}$$

where $\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3$ are named as the convected base vectors [15, 18]. Define the 9-dimensional vector

$$\boldsymbol{q}=\begin{bmatrix} \boldsymbol{q}_1^T & \boldsymbol{q}_2^T & \boldsymbol{q}_3^T \end{bmatrix}^T \tag{26}$$

and then the orthonormal constraints presented by (2), can be rewritten as

$$\boldsymbol{\psi}(\boldsymbol{q})=\begin{bmatrix} \frac{1}{2}(\boldsymbol{q}_1^T\boldsymbol{q}_1-1) \\ \frac{1}{2}(\boldsymbol{q}_2^T\boldsymbol{q}_2-1) \\ \frac{1}{2}(\boldsymbol{q}_3^T\boldsymbol{q}_3-1) \\ \frac{1}{2\sqrt{2}}(\boldsymbol{q}_2^T\boldsymbol{q}_3+\boldsymbol{q}_3^T\boldsymbol{q}_2) \\ \frac{1}{2\sqrt{2}}(\boldsymbol{q}_3^T\boldsymbol{q}_1+\boldsymbol{q}_1^T\boldsymbol{q}_3) \\ \frac{1}{2\sqrt{2}}(\boldsymbol{q}_1^T\boldsymbol{q}_2+\boldsymbol{q}_2^T\boldsymbol{q}_1) \end{bmatrix}=\mathbf{0} \tag{27}$$

Substituting (26) into (16) yields the expression of angular velocity

$$\begin{aligned} \Omega_1 &= (-\boldsymbol{q}_2^T\dot{\boldsymbol{q}}_3+\boldsymbol{q}_3^T\dot{\boldsymbol{q}}_2)/2 \\ \Omega_2 &= (-\boldsymbol{q}_3^T\dot{\boldsymbol{q}}_1+\boldsymbol{q}_1^T\dot{\boldsymbol{q}}_3)/2 \\ \Omega_3 &= (-\boldsymbol{q}_1^T\dot{\boldsymbol{q}}_2+\boldsymbol{q}_2^T\dot{\boldsymbol{q}}_1)/2 \end{aligned} \tag{28}$$

Correspondingly, the projection matrix is expressed as

$$\boldsymbol{L}(\boldsymbol{q})=\frac{1}{2}\begin{bmatrix} \mathbf{0} & -\boldsymbol{q}_3 & \boldsymbol{q}_2 \\ \boldsymbol{q}_3 & \mathbf{0} & \boldsymbol{q}_1 \\ -\boldsymbol{q}_2 & \boldsymbol{q}_1 & \mathbf{0} \end{bmatrix} \tag{29}$$

3 DYNAMICS AND INERTIA REPRESENTATIONS

In rigid body dynamics, the motion of a single body is governed by the Lagrange's equations of first kind. Suppose that the translation vector $\boldsymbol{x}_0 = \boldsymbol{0}$, and the equations of rotation motion can be expressed in a unified form

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{\boldsymbol{q}}}\right) - \frac{\partial T}{\partial \boldsymbol{q}} = \boldsymbol{Q} + \boldsymbol{Q}^c \tag{30}$$

In the above expression, $\boldsymbol{Q}$ denotes the generalized torque vector in terms of the generalized coordinates $\boldsymbol{q}$. Suppose that the rigid body is rotating in gravitational fields, the generalized torque vector can be expressed as

$$\boldsymbol{Q} = -\partial U / \partial \boldsymbol{q} \tag{31}$$

where U is the potential energy. The vector $\boldsymbol{Q}^c$ denotes the constrained forces. While minimal representation is implemented (e.g. Euler angles), $\boldsymbol{Q}^c$ is identically equal to zero, whereas the constrained forces are defined as

$$\boldsymbol{Q}^c = \boldsymbol{A}(\boldsymbol{q})^T \boldsymbol{\lambda} \tag{32}$$

where $\boldsymbol{A}$ is the constraint jacobian matrix, defined by

$$\boldsymbol{A}(\boldsymbol{q}) = \partial \boldsymbol{\psi}(\boldsymbol{q}) / \partial \boldsymbol{q}^T \tag{33}$$

and $\boldsymbol{\lambda}$ is the Lagrange's multiplier which preserves the path of pseudo-vector satisfying the constraints (12). Define the generalized momentum

$$\boldsymbol{p} = \partial T / \partial \dot{\boldsymbol{q}} = \boldsymbol{M}\dot{\boldsymbol{q}} \tag{34}$$

and the generalized force

$$\boldsymbol{f} = \partial T / \partial \boldsymbol{q} + \boldsymbol{Q} \tag{35}$$

and then Expression (30) can be expressed in a simplified form

$$\dot{\boldsymbol{p}} = \boldsymbol{f} + \boldsymbol{Q}^c \tag{36}$$

3.1 The modified inertia representation for rotation motion

The inertia representation, associated with mass matrix, establishes the connection between velocity of a system and the kinetic energy of that system. The mass matrix of a system is of various forms in representation: Firstly, it can be observed from the above that inertia representations of rotation motion are different if only different rotational coordinates, such as Euler angles, unit quaternion and convected base vectors, are implemented in practice; Secondly, the inertia representation is non-unique, even if the system is described under the same generalized coordinate. The former is a clear and logical conclusion, and the latter would be intensively investigated in the following, though it is not terribly intuitive in understanding.

Without loss of generality, suppose that the body-fixed coordinate axes $O\text{-}XYZ$ are aligned along the principal axes of inertia of the rigid body, and then the inertia tensor can be expressed as $\boldsymbol{J} = \text{diag}(J_1, J_2, J_3)$. Pre-multiply Expression (11) by itself, and then we have

$$\boldsymbol{\Omega}^T \boldsymbol{\Omega} = \dot{\boldsymbol{q}}^T \boldsymbol{L}(\boldsymbol{q}) \boldsymbol{L}(\boldsymbol{q})^T \dot{\boldsymbol{q}} \tag{37}$$

Assuming that

$$\dot{\boldsymbol{q}}^T \boldsymbol{L}(\boldsymbol{q})\boldsymbol{L}(\boldsymbol{q})^T \dot{\boldsymbol{q}} = \dot{\boldsymbol{q}}^T \dot{\boldsymbol{q}} \tag{38}$$

and then it can be derived that

$$\boldsymbol{\Omega}^T \boldsymbol{\Omega} = \dot{\boldsymbol{q}}^T \dot{\boldsymbol{q}} \tag{39}$$

Reformulate the rotational part of kinetic energy in an equivalent form

$$T = \frac{1}{2}\sigma \boldsymbol{\Omega}^T \boldsymbol{\Omega} + \frac{1}{2}\boldsymbol{\Omega}^T \boldsymbol{J}_\sigma \boldsymbol{\Omega} \tag{40}$$

where

$$\boldsymbol{J}_\sigma = \boldsymbol{J} - \sigma \boldsymbol{I}_3 \tag{41}$$

and $\sigma > 0$, and then substituting (11) and (39) into (40) yields a new type of formulation of kinetic energy

$$T = \frac{1}{2}\sigma \dot{\boldsymbol{q}}^T \dot{\boldsymbol{q}} + \frac{1}{2}\dot{\boldsymbol{q}}^T \boldsymbol{L}(\boldsymbol{q})\boldsymbol{J}_\sigma \boldsymbol{L}(\boldsymbol{q})^T \dot{\boldsymbol{q}} \tag{42}$$

In the modified inertia representation, the kinetic energy is generally split into a square term of velocity and a quadratic form in the derivatives with quadratic coefficients in generalized coordinates, of which the proportion is controlled by a scaling parameter, denoted as σ. Based on the Legendre transformation, we can derive the generalized momentum,

$$\boldsymbol{p} = \boldsymbol{M}_\sigma \dot{\boldsymbol{q}} \tag{43}$$

where

$$\boldsymbol{M}_\sigma = \sigma \boldsymbol{I} + \boldsymbol{L}(\boldsymbol{q})\boldsymbol{J}_\sigma \boldsymbol{L}(\boldsymbol{q})^T \tag{44}$$

and $\boldsymbol{I}$ is the identity matrix. The mass matrix $\boldsymbol{M}_\sigma$, presented by (44), is distinguished with the mass matrix $\boldsymbol{M}$ since an identity matrix with respect to the scaling parameter σ is separated from the original mass matrix, and while $\sigma = 0$, the two matrices are of the same formulations. Consequently, substituting (43) into (36), we can obtain a more generalized formulation of Lagrange's equations for rotation motion.

3.2 The inertia representations under different rotational coordinates

In the proceeding section, a newly inertia representation are derived by addition and subtraction of the homogeneous isotropic form $\frac{1}{2}\sigma \boldsymbol{\Omega}^T \boldsymbol{\Omega}$. It can be observed that the assumption presented by (38), plays an important role in the derivational process. However, this restriction is not a necessary condition to make sure the existence of the inertia representation, but it provides a clear way to reach the ultimate formulations, and the mass matrix presented by (44) can be considered as the standard formulation of mass matrix in the modified representation. Here we aim to develop the application of the modified inertia representation to three different rotational coordinates presented above.

1) Euler angles

While Euler angles is considered as the rotational coordinates, Pre-multiplying Expression (19) by itself and considering trigonometric identities yield

$$\boldsymbol{L}\boldsymbol{L}^T=\begin{bmatrix}1 & 0 & \cos\theta\\ 0 & 1 & 0\\ \cos\theta & 0 & 1\end{bmatrix} \tag{45}$$

Substituting (45) into (37) yields

$$\boldsymbol{\Omega}^T\boldsymbol{\Omega}=\dot{\boldsymbol{q}}^T\dot{\boldsymbol{q}}+2\dot{\psi}\dot{\phi}\cos\theta \tag{46}$$

Substitute (11) and (46) into (40) , and finally the mass matrix can be formally expressed as

$$\boldsymbol{M}_\sigma=\sigma\begin{bmatrix}1 & 0 & \cos\theta\\ 0 & 1 & 0\\ \cos\theta & 0 & 1\end{bmatrix}+\boldsymbol{L}(\boldsymbol{q})\boldsymbol{J}_\sigma\boldsymbol{L}(\boldsymbol{q})^T \tag{47}$$

2) Unit quaternion

While unit quaternion is considered as the rotational coordinates, the unit length constraint leads to

$$\dot{\boldsymbol{q}}^T\boldsymbol{q}=0 \tag{48}$$

Pre-multiplying Expression (24) by itself and considering $\boldsymbol{q}^T\boldsymbol{q}=1$ gives

$$\boldsymbol{L}(\boldsymbol{q})\boldsymbol{L}(\boldsymbol{q})^T=4\boldsymbol{I}_4-4\boldsymbol{q}\boldsymbol{q}^T \tag{49}$$

where $\boldsymbol{I}_4$ is 4-dimentional identity matrix. Substituting (48) and (49) into (37) yields

$$\boldsymbol{\Omega}^T\boldsymbol{\Omega}=4\dot{\boldsymbol{q}}^T\dot{\boldsymbol{q}} \tag{50}$$

Substitute (11) and (50) into (40) , and finally the mass matrix can be expressed as

$$\boldsymbol{M}_\sigma=4\sigma\boldsymbol{I}_4+\boldsymbol{L}(\boldsymbol{q})\boldsymbol{J}_\sigma\boldsymbol{L}(\boldsymbol{q})^T \tag{51}$$

3) Convected base vectors

While convected base vectors are considered as the rotational coordinates, the orthonormal constraints lead to the following constraint jacobian matrix

$$\boldsymbol{A}=\begin{bmatrix}\boldsymbol{q}_1 & \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} & \frac{1}{\sqrt{2}}\boldsymbol{q}_3 & \frac{1}{\sqrt{2}}\boldsymbol{q}_2\\ \boldsymbol{0} & \boldsymbol{q}_2 & \boldsymbol{0} & \frac{1}{\sqrt{2}}\boldsymbol{q}_3 & \boldsymbol{0} & \frac{1}{\sqrt{2}}\boldsymbol{q}_1\\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{q}_3 & \frac{1}{\sqrt{2}}\boldsymbol{q}_2 & \frac{1}{\sqrt{2}}\boldsymbol{q}_1 & \boldsymbol{0}\end{bmatrix}^T \tag{52}$$

The constraint jacobian matrix satisfies the following orthogonal relation

$$\boldsymbol{A}\dot{\boldsymbol{q}}=\boldsymbol{0} \tag{53}$$

A direct calculation reveals that

$$[\sqrt{2}\boldsymbol{L},\ \boldsymbol{A}^T]\begin{bmatrix}\sqrt{2}\boldsymbol{L}^T\\ \boldsymbol{A}\end{bmatrix}=\begin{bmatrix}\sqrt{2}\boldsymbol{L}^T\\ \boldsymbol{A}\end{bmatrix}[\sqrt{2}\boldsymbol{L},\ \boldsymbol{A}^T]=\boldsymbol{I}_9 \tag{54}$$

where $\boldsymbol{I}_9$ is 9-dimentional identity matrix. Substituting (53) and (54) into (37) gives

$$\boldsymbol{\Omega}^T \boldsymbol{\Omega} = \dot{\boldsymbol{q}}^T \dot{\boldsymbol{q}} / 2 \tag{55}$$

and hence, the mass matrix can be expressed as

$$\boldsymbol{M}_\sigma = \sigma \boldsymbol{I}/2 + \boldsymbol{L}(\boldsymbol{q}) \boldsymbol{J}_\sigma \boldsymbol{L}(\boldsymbol{q})^T \tag{56}$$

3.3 A glance about the error estimation

In the above, three different formulations of mass matrix has been derived for rotational motion under the modified representation, and a scaling parameter σ is formally, extracted from the original formulations. In the continuous case these formulations with different scaling parameter σ are theoretically equivalent, that specifically the scaling parameter can be eliminated if only one admits that the geometric relations, which should be obeyed by rotational coordinates for describing rotation motion, are precisely satisfied. However, this is not always reached by every kind of rotational coordinate in numerical simulation.

Suppose that $\boldsymbol{q} = \boldsymbol{q}(t)$ denotes the real solution of rotation motion of a single body, and $\boldsymbol{q}^+ = \boldsymbol{q}^+(t)$ is its numerical approximated solution. Correspondingly, we can define

$$\boldsymbol{L} = \boldsymbol{L}(\boldsymbol{q}), \quad \boldsymbol{L}^+ = \boldsymbol{L}(\boldsymbol{q}^+) \tag{57}$$

and

$$\boldsymbol{\Omega} = \boldsymbol{L}^T \dot{\boldsymbol{q}}, \ \boldsymbol{\Omega}^+ = (\boldsymbol{L}^+)^T \dot{\boldsymbol{q}}^+, \ \delta\boldsymbol{\Omega} = \boldsymbol{\Omega}^+ - \boldsymbol{\Omega} \tag{58}$$

Then the approximation error of kinetic energy can be expressed as

$$\delta T = T(\boldsymbol{q}^+, \dot{\boldsymbol{q}}^+) - T(\boldsymbol{q}, \dot{\boldsymbol{q}}) \tag{59}$$

Without loss of generality, we assume that the relation presented by (38), is satisfied, and then the kinetic energy can be expressed in the standard form under the modified representation of inertia. In combination of (57), (58) and (59) with (42), it can be derived that

$$\delta T = K_s \sigma + \delta T_0 \tag{60}$$

where

$$\delta T_0 = \delta \boldsymbol{\Omega}^T \boldsymbol{J} \boldsymbol{\Omega} + \delta \boldsymbol{\Omega}^T \boldsymbol{J} \delta \boldsymbol{\Omega} / 2 \tag{61}$$

is just the numerical error of the kinetic energy with the original formulation of kinetic energy, and the slope K_s is

$$K_s = \tfrac{1}{2}(\dot{\boldsymbol{q}}^{+T} \dot{\boldsymbol{q}}^+ - \boldsymbol{\Omega}^{+T} \boldsymbol{\Omega}^+) = \tfrac{1}{2} \dot{\boldsymbol{q}}^{+T} [\boldsymbol{I} - \boldsymbol{L}^+ (\boldsymbol{L}^+)^T] \dot{\boldsymbol{q}}^+ \tag{62}$$

It can be observed that the scaling parameter σ has no influence on the numerical error of kinetic energy if and only if $K_s = 0$, whereas the discretization error of kinetic energy is a linear function with respect to the scaling parameter.

While rotational coordinates are expressed in minimal representation, $K_s = 0$ is equivalent to $\boldsymbol{L}^+ (\boldsymbol{L}^+)^T = \boldsymbol{I}$. Consider that all the geometric relations are satisfied automatically in minimal representation, and this would not be broken by any perturbation about the rotational coordinates. Consequently, $\boldsymbol{L}^+ (\boldsymbol{L}^+)^T = \boldsymbol{I}$ if only $\boldsymbol{L}\boldsymbol{L}^T = \boldsymbol{I}$, and this assumption is admitted at the beginning of the discussion. As a result, we can conclude that the scaling parameter σ has no influence on the numerical error in minimal representation. For instance, we consider the Euler angles, that one of the minimal representation, as the rotational coordinates. In this case, the representation is not in standard form. However, a direct calculation reveals that

$$\boldsymbol{L}^{+}(\boldsymbol{L}^{+})^{T}=\begin{bmatrix}1 & 0 & \cos\theta^{+}\\ 0 & 1 & 0\\ \cos\theta^{+} & 0 & 1\end{bmatrix} \tag{63}$$

and this leads to

$$\boldsymbol{M}_{\sigma}^{+}=\sigma\boldsymbol{L}^{+}(\boldsymbol{L}^{+})^{T}+\boldsymbol{L}(\boldsymbol{q}^{+})\boldsymbol{J}_{\sigma}\boldsymbol{L}(\boldsymbol{q}^{+})^{T}=\boldsymbol{L}(\boldsymbol{q}^{+})\boldsymbol{J}\boldsymbol{L}(\boldsymbol{q}^{+})=\boldsymbol{M} \tag{64}$$

Hence the scaling parameter can be directly eliminated from the expression of mass matrix in minimal representation.

While rotational coordinates are expressed in non-minimal representation (i.e. the pseudo-vector), the geometric relations, which should be obeyed by rotational coordinates, are directly embodied as the constraints $\boldsymbol{\psi}(\boldsymbol{q})=\boldsymbol{0}$ and the implicit orthogonal relations $\boldsymbol{A}\dot{\boldsymbol{q}}=\boldsymbol{0}$. In continuous case, the scaling parameter σ can be eliminated from the formulation of kinetic energy through the geometric relation $\boldsymbol{\psi}(\boldsymbol{q})=\boldsymbol{0}$ and $\boldsymbol{A}\dot{\boldsymbol{q}}=\boldsymbol{0}$. Nevertheless, the geometric relations $\boldsymbol{\psi}(\boldsymbol{q})=\boldsymbol{0}$ can only be satisfied strictly at every time-grid points in the discretization process, following which the scaling parameter σ cannot be eliminated from the formulation of kinetic energy (i.e. $K_s\neq 0$), and consequently, the numerical accuracy of integration can be improved by determining a proper value of the scaling parameter σ. This distinguishes the modified representation of inertia with others in numerical significance. This numerical phenomenon is first discovered by Xu and Zhong [19] in their research about unit quaternion. They further recommend that

$$\sigma_{\mathrm{m}}=(J_1+J_2+J_3)/3 \tag{65}$$

is a reasonable preconditioning value for the scaling parameter. In the following, we will first develop the variational integrator for rigid body dynamics in pseudo-vector by considering the modified inertia representation, and further investigate the numerical performance of the scaling parameter σ through two numerical examples.

4 A DIRECT DISCRETIZING APPROACH FOR VARIATIONAL INTEGRATOR

Considered the generalized momentum defined by

$$\boldsymbol{p}=\boldsymbol{M}_{\sigma}(\boldsymbol{q})\dot{\boldsymbol{q}} \tag{66}$$

where $\boldsymbol{M}_{\sigma}$ is expressed specifically by (51) for unit quaternion and (56) for convected base vectors. Define an equidistant time grid, consisting of a number $N+1$ of discrete points t_k, defined by

$$t_k=k\Delta t \qquad k\in[0,1,\ldots,N] \tag{67}$$

Then differential part of the Lagrange's equations, presented by (36) can be formally written as

$$\dot{\boldsymbol{p}}_k=\boldsymbol{f}_k+\boldsymbol{Q}_k^{c} \tag{68}$$

for every discrete time $t_k=[0,N\Delta t]$. The approximation of the above equations leads to different difference schemes in Lagrange's frame. Here we define the difference approximations

$$\dot{\boldsymbol{q}}_{k+1/2} = (\boldsymbol{q}_{k+1} - \boldsymbol{q}_k)/\Delta t, \quad \boldsymbol{q}_{k+1/2} = (\boldsymbol{q}_k + \boldsymbol{q}_{k+1})/2 \tag{69}$$

and correspondingly, define

$$\boldsymbol{p}_{k+1/2} = \boldsymbol{M}_\sigma(\boldsymbol{q}_{k+1/2})\dot{\boldsymbol{q}}_{k+1/2}, \ \boldsymbol{f}_{k+1/2} = \boldsymbol{f}(\boldsymbol{q}_{k+1/2}, \dot{\boldsymbol{q}}_{k+1/2}) \tag{70}$$

Then the vectors $\dot{\boldsymbol{p}}_k$ and $\boldsymbol{f}_k$ are approximated as

$$\dot{\boldsymbol{p}}_k \approx (\boldsymbol{p}_{k+1/2} - \boldsymbol{p}_{k-1/2})/\Delta t \ , \quad \boldsymbol{f}_k \approx (\boldsymbol{f}_{k-1/2} + \boldsymbol{f}_{k+1/2})/2 \tag{71}$$

Substituting (32) and (71) into (68) and considering the constraint conditions (12) yield the following schemes

$$(\boldsymbol{p}_{k+1/2} - \boldsymbol{p}_{k-1/2})/\Delta t \ = (\boldsymbol{f}_{k-1/2} + \boldsymbol{f}_{k+1/2})/2 + s\boldsymbol{A}(\boldsymbol{q}_k)^T \tilde{\boldsymbol{\lambda}}_k, \quad \boldsymbol{\psi}(\boldsymbol{q}_{k+1}) = \boldsymbol{0} \tag{72}$$

where $\tilde{\boldsymbol{\lambda}} = \boldsymbol{\lambda}/s$ are scaled Lagrange multipliers and the scaling factor s can be set to any constant and is recommended as $s = \Delta t^{-2}$ to avoid ill-conditioning problem of iteration matrices [20]. The three-term recursion (72) is proposed by Leyendecker et al [21] through discrete variational principle (also see Wendlandt and Marsden [22]), and in the first step, it can be simplified to the term recursion

$$(\boldsymbol{p}_{1/2} - \boldsymbol{p}_0)/(\tfrac{1}{2}\Delta t) = \boldsymbol{f}_{1/2} + \tfrac{1}{2} s\boldsymbol{A}(\boldsymbol{q}_0)^T \tilde{\boldsymbol{\lambda}}_0, \ \boldsymbol{\psi}(\boldsymbol{q}_1) = \boldsymbol{0} \tag{73}$$

The specific algorithm is summarized in pseudo-code format in Table 1.

1)	Initial condition: $\boldsymbol{q}_0$, $\boldsymbol{p}_0$, $\tilde{\boldsymbol{\lambda}}_{-1} = \boldsymbol{0}$.
2)	Prediction step: $\boldsymbol{g}_{k+1} = \boldsymbol{g}_k$ where $\boldsymbol{g}_k = [\boldsymbol{q}_k^T \quad \tilde{\boldsymbol{\lambda}}_{k-1}]^T$
3)	Residual calculation: $\boldsymbol{r} = [\boldsymbol{r}_{\boldsymbol{q}} \quad \boldsymbol{r}_\lambda]^T$ $\begin{cases} \boldsymbol{r}_{\boldsymbol{q}} = (\boldsymbol{p}_{1/2} - \boldsymbol{p}_0)/(\tfrac{1}{2}\Delta t) - \boldsymbol{f}_{1/2} - \tfrac{1}{2} s\boldsymbol{A}(\boldsymbol{q}_0)^T \tilde{\boldsymbol{\lambda}}_0, k = 0 \\ \boldsymbol{r}_{\boldsymbol{q}} = (\boldsymbol{p}_{k+1/2} - \boldsymbol{p}_{k-1/2})/\Delta t - (\boldsymbol{f}_{k-1/2} + \boldsymbol{f}_{k+1/2})/2 - s\boldsymbol{A}(\boldsymbol{q}_k)^T \tilde{\boldsymbol{\lambda}}_k, \ k \ge 1 \end{cases}$ $\boldsymbol{r}_\lambda = \boldsymbol{\psi}(\boldsymbol{q}_{k+1})$
4)	Update incremental rotation parameters: $\delta\boldsymbol{g} = -\boldsymbol{K}^{-1}\boldsymbol{r}, \ \boldsymbol{g}_{k+1} = \boldsymbol{g}_k + \delta\boldsymbol{g}$, where $\boldsymbol{K} = \partial\boldsymbol{r}/\partial\boldsymbol{g}_{k+1}^{\mathrm{T}}$ and If $\lVert\boldsymbol{r}\rVert > \varepsilon_r$, repeat from 3).
5)	Return to 2) for new step, or stop.

Table 1: Variational integrator algorithm

5 NUMERICAL EXAMPLES

The numerical examples deal with a top spinning in gravitational field. As is shown in Figure 2, a top with the mass m is considered. The distance between mass center A and fixed point O is denoted by l, and the gravitational acceleration g is equal to 9.81 in the negative z-direction. While unit quaternion is considered, the gravitational potential energy of the top can be written as

$$U(\boldsymbol{q}) = mgl\cos\theta = mgl\boldsymbol{q}^T\boldsymbol{K}\boldsymbol{q} \tag{74}$$

where $\boldsymbol{K} = \mathrm{diag}(1, -1, -1, 1)$ and correspondingly, we have

$$\partial U/\partial \boldsymbol{q} = 2mgl\boldsymbol{K}\boldsymbol{q} \tag{75}$$

While convected base vectors are considered, the gravitational potential energy of the top can be written

$$U(\boldsymbol{q}) = mgl\cos(\theta) = ml\boldsymbol{g}^T\boldsymbol{q}_3 \tag{76}$$

where the gravitational vector is given as $\boldsymbol{g}^T = [0, 0, g]$. Hence external force can be expressed as

$$\partial U/\partial \boldsymbol{q} = [0 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0 \quad ml\boldsymbol{g}^T]^T \tag{77}$$

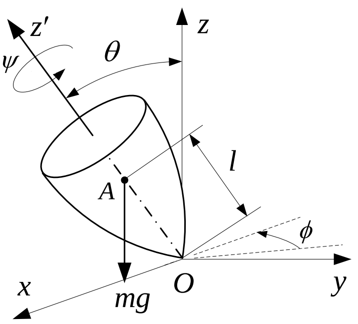

Figure 2: A heavy top.

5.1 Fast spinning top

Firstly, the fast spinning of a symmetric top is considered. The parameters are corresponding to $m=1$, $l=0.04$, and the principal moments of inertia tensor with respect to the fixed point $[J_1, J_2 = J_3] = [0.002, 0.0008]$. The following initial condition is considered

$$[\phi_0, \theta_0, \psi_0] = [0, \pi/6, 0], \quad \boldsymbol{\Omega}_0^T = [0, 0, 40\pi] \tag{78}$$

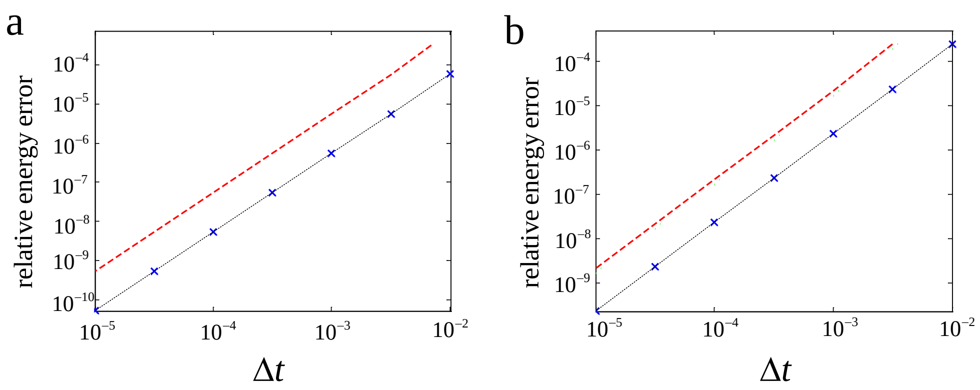

Figure 3: the maximum of periodic energy error with time step increasing. (a) unit quaternion, (b) convected base vectors. $\sigma = 0$ (---), $\sigma = \sigma_m$ (×).

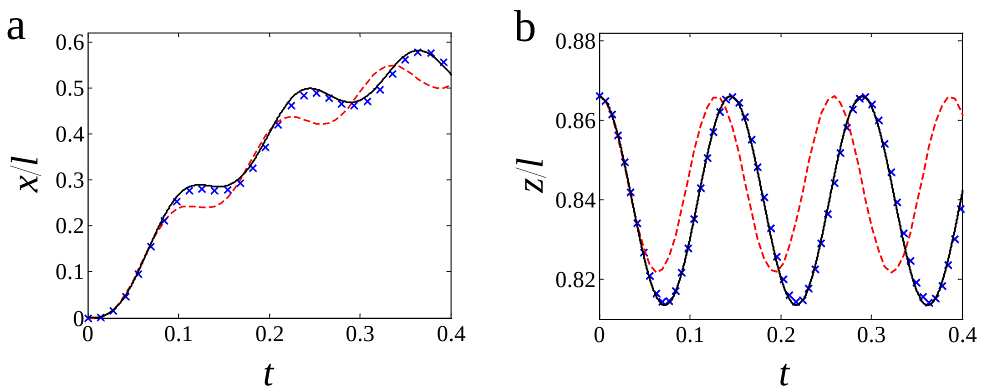

Figure 4: Trajectory errors of variational integrator with unit quaternion. (a) the x - component of mass center, (b) the z - component of mass center. $\sigma = 0$ (---), $\sigma = \sigma_m$ (×), analytical (—), time step $\Delta t = 0.007$.

Figures 3-5 show numerical comparison of variational integrators with different values of scaling parameter σ. Figure 3 presents that the variational integrator is a two-order algorithm. Figures 3-5 further present that the variational integrator with $\sigma = \sigma_m$ is of impressively higher accuracy than that with $\sigma = 0$. Considered that $\boldsymbol{M}_\sigma(\sigma = 0) = \boldsymbol{M}$, the value of the scaling parameter σ, in modified inertia representation, can greatly influence the numerical accuracy of integrations , although it can be determined arbitrarily in theoretical analysis.

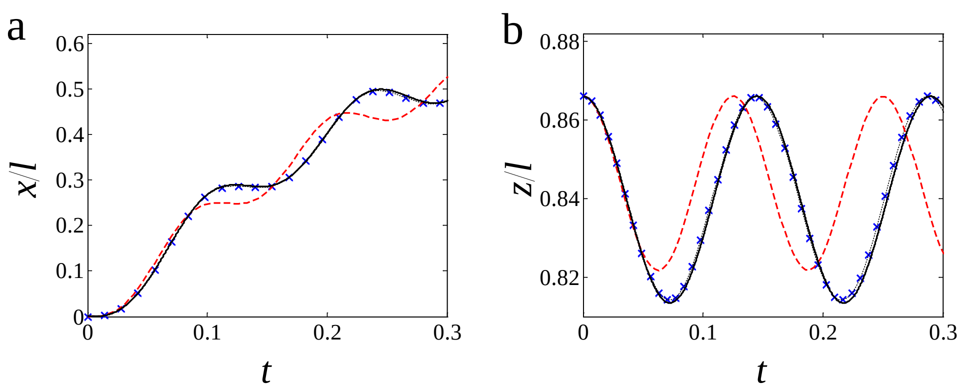

Figure 5: Trajectory errors of variational integrator with convected base vectors. (a) the x - component of mass center, (b) the z - component of mass center. $\sigma = 0$ (---), $\sigma = \sigma_m$ (×), analytical (—), time step $\Delta t = 0.0035$

5.2 Regular precession

We secondly consider the regular precession of a heavy top in gravitational field. The top is represented as a cone with dimensions equivalent to those used in [16-18]. As illustrated in Figure 2, the parameters are height $h = 0.1$, $l = \frac{3}{4}h$, radius $r = h/2$ and the mass $m = \rho\pi^2 h/3$ with the mass density $\rho = 2700$. The principal values of the inertia moments with respect to fixed point are given by

$$J_1 = J_2 = 0.6\, m(0.25r^2 + h^2), \quad J_3 = 0.3\, mr^2 \tag{79}$$

The regular precession requires that nutation angle θ, the velocity components $\dot{\phi}$ and $\dot{\psi}$ satisfy the relation

$$\dot{\psi} = (J_3\dot{\phi})^{-1}mgl + J_3^{-1}(J_1 - J_3)\dot{\phi}\cos(\theta) \tag{80}$$

see e.g. [1]. The initial conditions correspond to those used in [16-18], i.e. a precession rate $\dot{\phi} = 10$, an initial nutation angle $\theta_0 = \pi/3$ and the initial angular velocity vector

$$\boldsymbol{\Omega}_0 = [0, \dot{\phi}\sin(\theta_0), \dot{\psi} + \dot{\phi}\cos(\theta_0)]^T \tag{81}$$

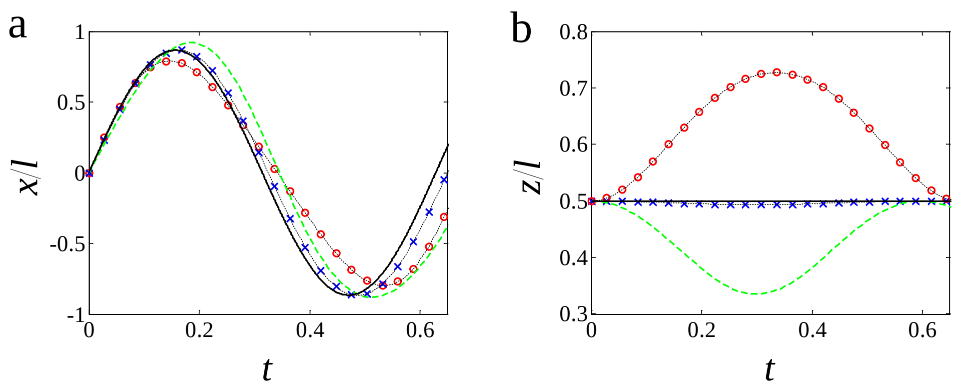

Figure 6: Numerical integrations with unit quaternion. (a) the x - component of mass center, (b) the z - component of mass center. Variational integrator with $\sigma = 0$ (∘) and $\sigma = \sigma_m$ (×), energy-momentum conserving scheme (---), analytical solution (—), time step $\Delta t = 0.01$.

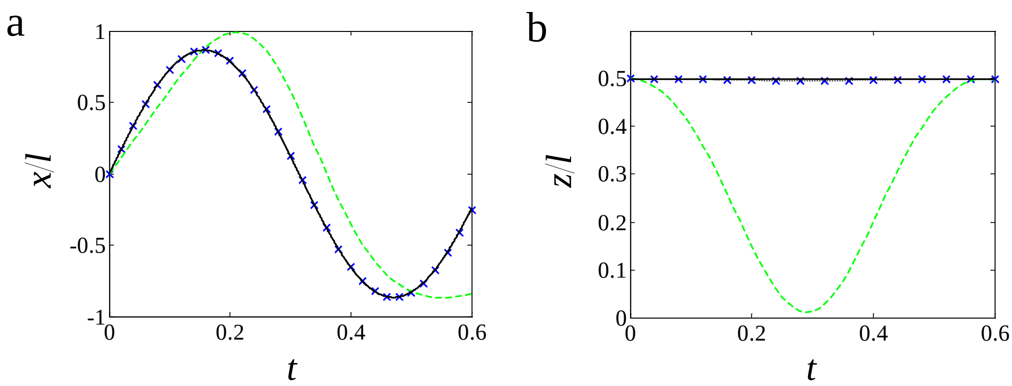

Figure 7: Numerical integrations with convected base vectors. (a) the x - component of mass center, (b) the z - component of mass center. Variational integrator with $\sigma = \sigma_m$, energy-momentum conserving scheme (---), analytical solution (—), time step $\Delta t = 0.01$.

Recently, regular precession top is detailed discussed by Krenk and Nielsen, in their researches about energy-momentum conserving integrations of rigid body dynamics [17,18]. They observed that the numerical integrations are of significant nutation error in simulation of regular precession, whether the integrations are implemented in terms of unit quaternion or convected base vectors. Figures 6-7 compare the numerical results of regular precession between the variational integrator and energy-momentum conserving schemes proposed by Krenk and Nielsen [17, 18]. It should be mentioned that the convected-base-vectors-based variational integrator with $\sigma = 0$ and $\Delta t = 0.01$ presents almost wrong numerical results in simulation, and hence is not shown in Figure 7. In addition, the energy-momentum schemes are implemented in terms of unit quaternion and convected base vector in Figures 6 and 7, respectively. It can be observed that the variational integrator with $\sigma = 0$ and energy-momentum conserving integration both present significant numerical errors, whereas the variational integrator with $\sigma = \sigma_{\mathrm{m}}$ present impressively high accuracy in simulation. In combination of Figures 6-7 with Figures 3-5, we can conclude that the numerical accuracy of integrations can be improved in modified representation of inertia, associated with the scaling parameter σ, and the mean value of three principal moments of inertia tensor can be considered as a reasonable value of the scaling parameter, with which the numerical integrations are expected to present much higher accuracy than others.

6 CONCLUSIONS

A modified inertia representation is proposed for rigid body dynamics, through splitting the kinetic energy into two parts, that a square term of velocity and a quadratic form in the derivatives with quadratic coefficients in generalized displacement. The proportion of the two components is controlled by a scaling parameter, denoted as σ. The associated mass matrix with different values of scaling parameter, are theoretically equivalent in dynamics. However, it presents different features while discretizing the govern equations of the system. Error estimation demonstrates that the discretization error of kinetic energy is a linear function with respect to the scaling parameter, of which the slope is not equal to zero if only the rotational coordinates are expressed in pseudo-vector, such as unit quaternion, convected base vectors, etc.

Error estimation implies that the numerical accuracy of integration can be improved by optimizing the scaling parameter. Based on the modified representation of inertia, a variational integrator is proposed for rigid body dynamics in terms of pseudo vectors. Two examples that the fast spinning top and the regular precession, are considered to testing the numerical performance of the scaling parameter. Numerical results demonstrate that the variational integrator with $\sigma=\sigma_{\mathrm{m}}$ presents impressively higher accuracy in simulation than other integrations. Consequently, the arithmetic mean value of the principal moments of inertia tensor (i.e. σ_{m}), is a reasonable preconditioning value of the scaling parameter, with which the numerical integrations are expected to present much higher accuracy than others.

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